

*Citation for published version:*

Hill, A & Norton, T 2015, 'An iterative starting method to control parasitism for the Leapfrog method', *Applied Numerical Mathematics*, vol. 87, no. 1, Volume 87, pp. 145.

*Publication date:*  
2015

*Document Version*  
Early version, also known as pre-print

[Link to publication](#)

**University of Bath**

## **Alternative formats**

If you require this document in an alternative format, please contact:  
[openaccess@bath.ac.uk](mailto:openaccess@bath.ac.uk)

### **General rights**

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

### **Take down policy**

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

See discussions, stats, and author profiles for this publication at: <http://www.researchgate.net/publication/266320292>

# An iterative starting method to control parasitism for the Leapfrog method

ARTICLE *in* APPLIED NUMERICAL MATHEMATICS · JANUARY 2014

Impact Factor: 1.04 · DOI: 10.1016/j.apnum.2014.09.005

---

DOWNLOADS

2

---

VIEWS

13

2 AUTHORS, INCLUDING:



[Adrian T. Hill](#)

University of Bath

24 PUBLICATIONS 190 CITATIONS

SEE PROFILE

# An iterative starting method to control parasitism in multivalued methods

Terence J. T. Norton<sup>a,\*</sup>, Adrian T. Hill<sup>a</sup>

<sup>a</sup>*Department of Mathematical Sciences, University of Bath, Bath BA2 7AY, United Kingdom*

---

## Abstract

Leapfrog is a time-symmetric method, widely used to solve the Euler equations and other Hamiltonian systems, due to its low cost and geometric properties. A difficulty with Leapfrog is that it suffers from parasitism. The severity of the parasitism is a function of the differential equation, the method and the time-step. When the tendency to parasitic growth is mild, this paper shows that the perceptible onset of parasitism may be delayed over long time-intervals, if parasitic components are attempted to be eliminated in the starting method. In theory, the ideal starting method corresponding to the underlying one-step method has no parasitic components. In practice, the paper describes how the ideal starter may be approximated iteratively. Leapfrog and the iterative starting procedure are applied to the cubic Schrödinger equation. Soliton behaviour is well-preserved over long time-intervals, as is the Hamiltonian.

*Keywords:* Parasitism, Starting method, Leapfrog, Cubic Schrödinger equation

---

## 1. Introduction

This paper investigates the influence of starting methods on parasitism for the Leapfrog method, applied to Hamiltonian and other integrable systems. Parasitism afflicts all linear multistep methods [?] and all explicit general linear methods possessing either the time-symmetric or  $G$ -symplectic property [?]. This is unfortunate, since such methods would otherwise be excellent candidates for efficient geometric integration.

Although Dahlquist [?] identified and analysed the problem of parasitism early in the computer era, he also observed that it is a relatively weak instability. In the particular case of the Leapfrog method, the weakness of this instability has led to a number of attempts to control it. One of the earliest such attempts was the Gragg smoother [?], which uses a finishing method to eliminate the leading order parasitic term. The Leapfrog method is also extensively used in Meteorology, where parasitism is controlled either by intermittent implicit steps, or by introducing a small amount of damping at each step; e.g. RAW filter [?]. Fornberg and Sanz-Serna and Vadillo

Shampine [?] recently suggested periodic restarts as a means to control parasitism in the Leapfrog method.

In this paper, we propose to control parasitism by attempting to . It is known [?, pp. 610-611] that a time-symmetric or  $G$ -symplectic multivalued method,  $\mathcal{M}_h$ , possesses an underlying one-step method  $\Phi_h$ , and that there is an ideal starting method  $\mathcal{S}_h^*$  such that

$$\mathcal{M}_h \mathcal{S}_h^* = \mathcal{S}_h^* \Phi_h.$$

If the computational starting method is equal to  $\mathcal{S}_h^*$  to high accuracy and  $\mathcal{F}_h$  is a suitable finishing method, then the computed numerical solution is equal to

$$\mathcal{F}_h \mathcal{M}_h^n \mathcal{S}_h^*(y_0) = \Phi_h^n(y_0).$$

---

\*Corresponding author

Email addresses: `tjtn20@bath.ac.uk` (Terence J. T. Norton), `masath@bath.ac.uk` (Adrian T. Hill)

The right-hand side of this identity is governed by repeated compositions of  $\Phi_h$ , rather than  $\mathcal{M}_h$ . Since  $\Phi_h$  is a one-step method, parasitism plays no part, in exact arithmetic.

The paper is organised as follows: In Section 2, we study how effective some simple starting methods are at controlling parasitism for the Leapfrog method applied to the simple pendulum problem. Best results are obtained for a simple symmetric method. In Section 3, we introduce general linear methods (GLMs). In Section 4, an iterative algorithm to construct an approximation to an ideal starting method  $\mathcal{S}_h^*$ , is described within the framework of general linear methods. In Section 5, the cubic Schrödinger equation is approximated using Leapfrog and the iterative starting algorithm initialised using the simple symmetric starting method of Section 2. Soliton behaviour is well-preserved over long time-intervals, as is the Hamiltonian.

## 2. A comparison of starting methods for the Leapfrog Method

Consider the autonomous initial value problem (IVP):

$$\frac{dy}{dt}(t) = f(y(t)), \quad y(0) = y_0, \quad t \in [0, T], \quad (1)$$

where  $f : X \rightarrow X$ ,  $y(t), y_0 \in X$  and  $T > 0$ . Associated with the solution  $y(t)$  is the *flow map*  $\varphi_t : X \rightarrow X$  such that

$$y(t) = \varphi_t(y_0), \quad t \in [0, T].$$

In this paper, we consider a Hamiltonian IVP defined on the space  $X = \mathbb{R}^{2d}$ ,  $d \in \mathbb{N}$  (see e.g. [? ]):

$$\frac{dy}{dt}(t) = J^{-1} \nabla_y H(y(t)) =: f(y(t)), \quad J^{-1} = \begin{bmatrix} 0 & -I_d \\ I_d & 0 \end{bmatrix}, \quad y(0) = y_0, \quad t \in [0, T], \quad (2)$$

where  $H : X \rightarrow \mathbb{R}$  is the Hamiltonian.

The Leapfrog method applied to IVP (1) is given by

$$U_{n+2} = U_n + 2hf(U_{n+1}), \quad n \in \mathbb{N}_0, \quad (3)$$

where  $h \in \mathbb{R} \setminus \{0\}$  is fixed and  $U_n \approx y(nh)$ . The method is time-symmetric and  $G$ -symplectic [? ], properties that are helpful in the integration of conservative systems. It is also second-order, i.e.

$$U_n = y(nh) + O(h^2), \quad 0 \leq n \leq \frac{T}{h}, \quad (4)$$

provided the starting values  $U_0, U_1 \in X$  are computed such that (4) holds for  $n = 0, 1$ . For example, consider the following three starting methods:

$$\textbf{Euler:} \quad \begin{cases} U_1 = y_0 + hf(y_0), \\ U_0 = y_0. \end{cases} \quad (5)$$

$$\textbf{Modified Euler:} \quad \begin{cases} U_1 = y_0 + \frac{h}{2}f(y_0) + \frac{h}{2}f(y_0 + hf(y_0)), \\ U_0 = y_0. \end{cases} \quad (6)$$

$$\textbf{Symmetric:} \quad \begin{cases} \tilde{U}_1 = y_0 + \frac{h}{2}f(y_0), \\ \tilde{U}_0 = y_0 - \frac{h}{2}f(y_0). \end{cases} \quad (7)$$

For the Euler and modified Euler starting methods, Gragg [? ] proved that the global error expansion for the Leapfrog method contains only even powers of  $h$ ; such expansions are characteristic of time-symmetric multistep methods [? , pp. 415-416].

The non-classical symmetric starting approximation produces inputs that do not approximate  $\varphi_h(y_0)$  and  $y_0$ . Thus, we require a finishing method, applied at the end of a step, to obtain approximations to  $y(nh)$ . In this case, an average of the components will suffice, i.e.

$$U_n = \frac{1}{2}(\tilde{U}_{n+1} + \tilde{U}_n), \quad (8)$$

where the  $\tilde{U}_n$  are obtained with the usual Leapfrog update.

**Example 2.1.** Consider the simple pendulum problem:

$$\frac{d}{dt} \begin{bmatrix} p(t) \\ q(t) \end{bmatrix} = \begin{bmatrix} -\sin(q(t)) \\ p(t) \end{bmatrix}, \quad \begin{bmatrix} p(0) \\ q(0) \end{bmatrix} = \begin{bmatrix} 1.0 \\ 2.0 \end{bmatrix}, \quad t \in [0, T], \quad T > 0. \quad (9)$$

We note that this is a Hamiltonian IVP, with a separable Hamiltonian of the form

$$H(q, p) = \frac{1}{2}p^2 - \cos(q).$$

We solve IVP (9) using the Leapfrog method initialised with each of the starting methods described above. In each case we use a fixed time-step of  $h = 0.1$ . For the Euler starting method we take  $T = 4$ ; for the modified Euler starting method we take  $T = 1000$ , and for the symmetric starting method we take  $T = 2000$ .

A comparison of Hamiltonian error,  $H(q_n, p_n) - H(q_0, p_0)$ , is given in Figure 1. The results for the Euler starting method, given in Figure 1a, show that the Hamiltonian is almost constant for about 10 time-steps. However, subsequently, the growth of a parasitic mode of the Leapfrog method overwhelms the principal component of the numerical solution. A similar experiment is performed in [?] where parasitism is also observed.

The numerical results for the modified Euler are displayed in Figure 1b. We find that the Hamiltonian is quite well-preserved for  $t \in [0, 50]$ . However, subsequently, parasitic instability begins to dominate the Hamiltonian error.

The results of the symmetric starting method are given in Figure 1c. While we find that the interval of good preservation has been further extended, parasitism ultimately dominates.

◇

### 2.1. Parasitism

From the previous experiments, we observe that parasitism is an inherent feature of the Leapfrog method. A basic explanation for this phenomenon may be obtained if we consider a perturbation to the  $n^{\text{th}}$  step in the direction of the eigenvector corresponding to the root  $\zeta = -1$  of the method's characteristic polynomial  $\rho(\zeta) = \zeta^2 - 1$ :

$$U_n \mapsto U_n + (-1)^n z_n.$$

Substituting this into the Leapfrog method (3) yields

$$\begin{aligned} U_{n+2} + (-1)^{n+2} z_{n+2} &= U_n + (-1)^n z_n + 2hf(U_{n+1} + (-1)^{n+1} z_{n+1}), \\ \Rightarrow z_{n+2} &= z_n + 2\mu h \nabla f(U_{n+1}) z_{n+1} + O(h \|z_{n+1}\|^2), \quad \forall n \geq 0, \end{aligned}$$

where  $\mu = -1$  is termed the *growth parameter*. An application of the discrete Gronwall lemma implies that

$$\|z_n\| \leq C(z_0, z_1) \exp(Lnh), \quad (10)$$

where  $L$  is a bound on  $\|\nabla f(\cdot)\|$  and  $C(z_0, z_1)$  is a constant depending on initial perturbations  $z_0, z_1$ .

The above analysis suggests that perturbations will corrupt the numerical solution over a time-scale of  $t = nh = O(1)$ . However, while our examples do show parasitic behaviour, good Hamiltonian preservation

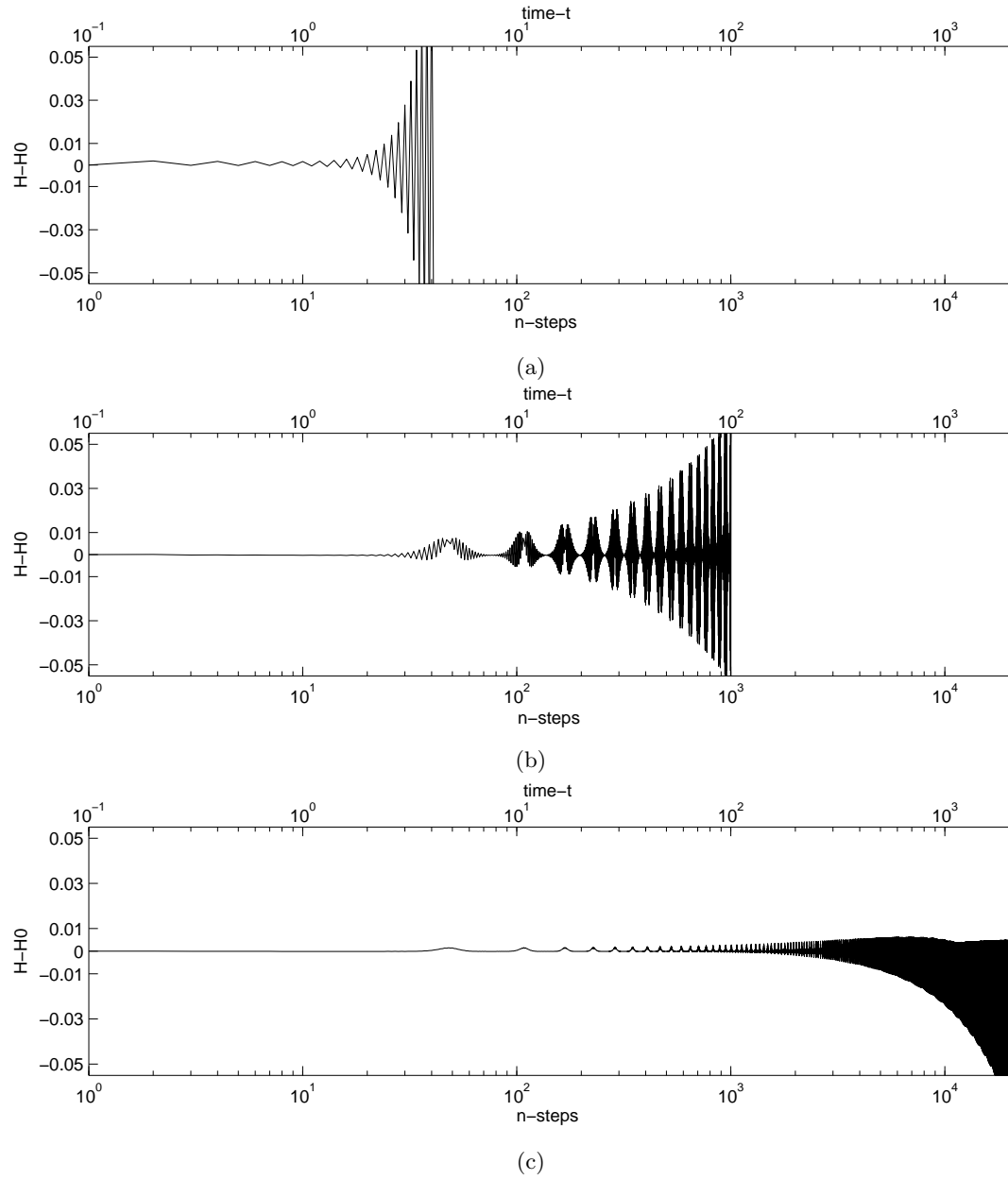


Figure 1: A comparison of Hamiltonian error for IVP (9) when integrating with the Leapfrog method (a) using the Euler starting method (5). (b) using the modified Euler starting method (6). (c) using the symmetric starting method (7) and finishing method (8).

is observed over modest time intervals. Therefore, estimate (10) should not necessarily be taken as a quantitative estimate of the interval of good behaviour, but as a qualitative indication.

Example 2.1 shows that starting methods can have a significant effect on the length of the time interval for which parasitism is relatively insignificant. This motivates our search for an improved starting method to extend the interval of good preservation.

### 3. General Linear Methods

It is our intention to construct a starting method that vastly increases the interval of good preservation. Our approach requires that we work within the GLM framework where non-classical starting and finishing methods arise naturally. We begin by reviewing the fundamental theory of GLMs [? ].

#### 3.1. Introduction to GLMs

A GLM may be seen as a generalisation of both Runge-Kutta methods and LMMs, i.e. multivalued-multistage methods. Each consists of  $r \in \mathbb{N}$  inputs and  $s \in \mathbb{N}$  stage evaluations. Numerical quantities  $y_i^{[n]} \in X$ ,  $i = 1, \dots, r$ , are generated via stage and update equations:

$$Y_i = h \sum_{j=1}^s a_{ij} f(Y_j) + \sum_{j=1}^r u_{ij} y_j^{[n]}, \quad i = 1, \dots, s \quad [\text{Stage Equations}],$$

$$y_i^{[n+1]} = h \sum_{j=1}^s b_{ij} f(Y_j) + \sum_{j=1}^r v_{ij} y_j^{[n]}, \quad i = 1, \dots, r \quad [\text{Update Equations}],$$

where  $Y_i \in X$  and  $a_{ij}, b_{ij}, u_{ij}, v_{ij} \in \mathbb{R}$  denote the method coefficients. For notational convenience, we define super-vectors

$$y^{[n+1]} = \begin{bmatrix} y_1^{[n+1]} \\ y_2^{[n+1]} \\ \vdots \\ y_r^{[n+1]} \end{bmatrix}, \quad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix}, \quad Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{bmatrix}, \quad F = \begin{bmatrix} f(Y_1) \\ f(Y_2) \\ \vdots \\ f(Y_s) \end{bmatrix},$$

and matrices

$$A = [a_{ij}] \in \mathbb{R}^{s \times s}, \quad B = [b_{ij}] \in \mathbb{R}^{r \times s}, \quad U = [u_{ij}] \in \mathbb{R}^{s \times r}, \quad V = [v_{ij}] \in \mathbb{R}^{r \times r}.$$

Then, the stage and update equations may be more compactly written as

$$\begin{bmatrix} Y \\ y^{[n+1]} \end{bmatrix} = \begin{bmatrix} A \otimes I_X & U \otimes I_X \\ B \otimes I_X & V \otimes I_X \end{bmatrix} \begin{bmatrix} hF \\ y^{[n]} \end{bmatrix}.$$

The coefficient matrices  $(A, U, B, V)$  characterise each GLM and we refer to a method using its *GLM tableau*

$$\begin{bmatrix} A & U \\ B & V \end{bmatrix}.$$

Below, we consider the map defined by the method:

**Definition 3.1.** A GLM with coefficient matrices  $(A, U, B, V)$  determines a map  $\mathcal{M}_h : X^r \rightarrow X^r$  which is defined by

$$Y = hAF + Uy^{[n]}, \\ \mathcal{M}_h(y^{[n]}) = hBF + Vy^{[n]},$$

where Kronecker products are taken as implied.

**Example 3.1.** The Leapfrog method (3) may be viewed as an  $s = 1, r = 2$  GLM:

$$\begin{aligned} \begin{bmatrix} U_{n+2} \\ U_{n+1} \end{bmatrix} &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} U_{n+1} \\ U_n \end{bmatrix} + 2h \begin{bmatrix} f(U_{n+1}) \\ 0 \end{bmatrix}, \\ &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} U_{n+1} \\ U_n \end{bmatrix} + h \begin{bmatrix} 2 \\ 0 \end{bmatrix} f \left( \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} U_{n+1} \\ U_n \end{bmatrix} \right). \end{aligned}$$

This may be rewritten as

$$y^{[n+1]} = Vy^{[n]} + hBf(Uy^{[n]}), \quad y^{[n]} := \begin{bmatrix} U_{n+1} \\ U_n \end{bmatrix},$$

for

$$U = \begin{bmatrix} 1 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 2 \\ 0 \end{bmatrix}, \quad V = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Thus, the GLM tableau of Leapfrog is given as

$$\begin{bmatrix} A & U \\ B & V \end{bmatrix} = \left[ \begin{array}{c|cc} 0 & 1 & 0 \\ 2 & 0 & 1 \\ 0 & 1 & 0 \end{array} \right].$$

◇

As with LMMs, we require a starting method to compute  $y^{[0]}$ . However, for GLMs, starting values do not necessarily have to be approximations to  $\varphi_{jh}(y_0)$ ,  $j = 0, \dots, r-1$ , rather as we have seen in Section 2 with starting method (7). As a result, we will also need to apply a finishing method. These methods are defined as follows:

**Definition 3.2.** A *starting method* is defined to be the map  $\mathcal{S}_h : X \rightarrow X^r$ , where

$$\mathcal{S}_h(y_0) = y^{[0]}.$$

A *finishing method* is defined to be the map  $\mathcal{F}_h : X^r \rightarrow X$  such that

$$\mathcal{F}_h(y^{[n]}) \approx y(nh), \quad \mathcal{F}_h \circ \mathcal{S}_h(y_0) = y_0, \quad \forall y_0 \in \mathbb{X}.$$

The numerical approximations to our ODE are given by the composite map  $\mathcal{F}_h \circ \mathcal{M}_h^n \circ \mathcal{S}_h(y_0)$ .

### 3.2. Convergence, Consistency & Stability

To guarantee convergence of a GLM we ensure that it is both *consistent* and *stable* [?]. We say that a GLM with real coefficient matrices  $(A, U, B, V)$  is

(a) *Preconsistent*, if  $(1, u)$  is an eigenpair of  $V$ , such that

$$Vu = u, \quad w^T u = 1;$$

for some  $w \in \mathbb{X}^r$ .

(b) *Consistent*, if it is preconsistent,  $Uu = \mathbb{1}$ , and  $\exists v \in \mathbb{R}^r \setminus \{0\}$  such that  $B\mathbb{1} + Vv = u + v$ , for  $\mathbb{1} = [1, 1, \dots, 1] \in \mathbb{R}^s$ .

(c) *Stable*, if it is *zero-stable*, i.e.

$$\sup_{n \geq 0} \|V^n\| < \infty,$$



### 3.3. Order

The order of a GLM can be expressed in terms of the pair  $(\mathcal{M}_h, \mathcal{S}_h)$ . Specifically, we say a GLM is of order  $p \in \mathbb{N}$  if

$$\mathcal{M}_h \circ \mathcal{S}_h(y_0) = \mathcal{S}_h \circ \varphi_h(y_0) + C(y_0)h^{p+1} + O(h^{p+2}), \quad (11)$$

where  $C(y_0)$  is constant depending on  $y_0$  and the method. The maximal order of a GLM is given by the highest order over all feasible  $\mathcal{S}_h$ . Note also that an application of a corresponding finishing method gives

$$\mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h(y_0) = \varphi_h(y_0) + O(h^{p+1}). \quad (12)$$

## 4. Iterative Starting Method

### 4.1. Underlying one-step map

The design of our iterative starting method relies on the connection between a GLM and its underlying one-step map.

**Definition 4.1 (Underlying one-step map).** The map  $\Phi_h : X \rightarrow X$  is called an *underlying one-step map* (UOSM) of a GLM if it satisfies

$$\mathcal{M}_h \circ \mathcal{S}_h^*(y_0) = \mathcal{S}_h^* \circ \Phi_h(y_0), \quad \forall y_0 \in X, \quad (13)$$

where  $\mathcal{S}_h^*$  is a corresponding consistent starting method.

Note that the application of a finishing method to (13) finds  $\Phi_h(y_0) = \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^*(y_0)$ , where  $\mathcal{F}_h \circ \mathcal{S}_h^*(y_0) = y_0$ . Properties of the UOSM are inherited from  $\mathcal{M}_h$ . For example, a time-symmetric or  $G$ -symplectic GLM yields a time-symmetric or conjugate-symplectic UOSM [? ? ].

The formal existence of the UOSM and  $\mathcal{S}_h^*$  has been shown, for example, in [? , pp. 610-611]. The statement of the result is given below:

**Theorem 4.1.** *Consider a consistent GLM. Furthermore, let  $\mathcal{M}_h(y^{[n]})$  and  $\mathcal{F}_h(y^{[n]}) = w^T y^{[n]} + \dots$ , have formal B-series expansions. Then, there exist a unique formal one-step method*

$$\Phi_h(y_0) = y_0 + h d_1(y_0) + h^2 d_2(y_0) + \dots,$$

*and a unique formal starting method*

$$\mathcal{S}_h^*(y_0) = w y_0 + h \mathcal{S}_1^*(y_0) + h^2 \mathcal{S}_2^*(y_0) + \dots, \quad (14)$$

*such that (13) and  $\mathcal{F}_h \circ \mathcal{S}_h^*(y_0) = y_0$  hold formally.*

Consider the ideal situation in which  $\mathcal{S}_h^*$  and  $\Phi_h$  converge to well-defined maps on  $X$ . Then,

$$\mathcal{F}_h \circ \mathcal{M}_h^n \circ \mathcal{S}_h^*(y_0) = \mathcal{F}_h \circ \mathcal{S}_h^* \circ \Phi_h^n(y_0) = \Phi_h^n(y_0).$$

In other words, a numerical solution obtained from a GLM is equivalent to that obtained from the UOSM. An important consequence is that the GLM will not suffer from parasitism, in exact arithmetic, since the UOSM is parasitism-free. In practice, the construction of  $\mathcal{S}_h^*$  is infeasible as (14) represents an infinite B-series with unknown convergence [? , pp. 575-576]. That being said, a high order approximation to  $\mathcal{S}_h^*$  may be sufficient to allow the UOSM to dominate the behaviour of the numerical solution, and to suppress parasitism over very long times.

#### 4.2. Iterative starting method

The principal idea behind the iterative starting method is similar to that of residual correction for an eigenvalue problem. We begin by introducing  $S$ ; the space of starting methods corresponding to  $\mathcal{M}_h$ . Then, we define maps  $\varepsilon : S \times X \rightarrow X^r$  and  $\eta : S \times X \rightarrow X$  such that

$$\begin{aligned}\eta(\mathcal{S}_h, y_0) &:= \mathcal{F}_h \circ \mathcal{S}_h(y_0) - y_0, \\ \varepsilon(\mathcal{S}_h, y_0) &:= \mathcal{M}_h \circ \mathcal{S}_h(y_0) - \mathcal{S}_h \circ \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h(y_0) + u \circ \eta(\mathcal{S}_h, y_0),\end{aligned}$$

for some fixed  $\mathcal{F}_h$ . The iterative starting method is given as

$$\begin{aligned}\mathcal{S}_h^{[k+1]}(y_0) &= \mathcal{S}_h^{[k]}(y_0) + D\varepsilon(\mathcal{S}_h^{[k]}, y_0) - u \circ \eta(\mathcal{S}_h^{[k]}, y_0), \quad \forall k \geq 0, \\ \mathcal{S}_h^{[0]}(y_0) &= \mathcal{S}_h(y_0),\end{aligned}$$

where

$$D = (I - uw^T)(I - V + uu^T)^{-1},$$

and  $\mathcal{F}_h$  is chosen to satisfy  $\mathcal{F}_h \circ \mathcal{S}_h(y_0) = y_0$ .

**Theorem 4.2.** *Suppose the pair  $(\mathcal{M}_h, \mathcal{S}_h)$  is of order  $p \in \mathbb{N}$  and  $\mathcal{F}_h$  is chosen such that  $\mathcal{F}_h \circ \mathcal{S}_h(y_0) = y_0$ . Then,*

$$\eta(\mathcal{S}_h^{[k]}, y_0) = \varepsilon(\mathcal{S}_h^{[k]}, y_0) = O(h^{k+p+1}), \quad \forall k \geq 0.$$

*Proof (by induction).* Let  $P(k)$  denote our inductive hypothesis:  $\eta(\mathcal{S}_h^{[k]}, y_0) = \varepsilon(\mathcal{S}_h^{[k]}, y_0) = O(h^{k+p+1})$  for  $k \geq 0$ .

( $k = 0$ ). Here,  $\eta(\mathcal{S}_h, y_0) = \mathcal{F}_h \circ \mathcal{S}_h(y_0) - y_0 = 0$ . From the order equations (11) & (12) we are given that

$$\mathcal{M}_h \circ \mathcal{S}_h(y_0) = \mathcal{S}_h \circ \varphi_h(y_0) + O(h^{p+1}) \quad \text{and} \quad \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h(y_0) = \varphi_h(y_0) + O(h^{p+1}).$$

Thus,

$$\begin{aligned}\varepsilon(\mathcal{S}_h, y_0) &= \mathcal{M}_h \circ \mathcal{S}_h(y_0) - \mathcal{S}_h \circ \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h(y_0) + u \circ \eta(\mathcal{S}_h, y_0), \\ &= \mathcal{M}_h \circ \mathcal{S}_h(y_0) - \mathcal{S}_h \circ \varphi_h(y_0) + O(h^{p+1}) = O(h^{p+1}).\end{aligned}$$

*Inductive Step.* Given  $P(m)$  for  $m \geq 0$ , we have that

$$\eta(\mathcal{S}_h^{[m+1]}, y_0) = \mathcal{F}_h \circ \mathcal{S}_h^{[m+1]}(y_0) - y_0 = \mathcal{F}_h \circ (\mathcal{S}_h^{[m]}(y_0) + D\varepsilon(\mathcal{S}_h^{[m]}, y_0) - u \circ \eta(\mathcal{S}_h^{[m]}, y_0)) - y_0.$$

The Fréchet derivative of  $\mathcal{F}_h$  is  $w^T + O(h)$  where  $w^T u = 1$ . Thus,

$$\begin{aligned}\eta(\mathcal{S}_h^{[m+1]}, y_0) &= (\mathcal{F}_h \circ \mathcal{S}_h^{[m]}(y_0) - y_0) - \eta(\mathcal{S}_h^{[m]}, y_0) + w^T D\varepsilon(\mathcal{S}_h^{[m]}, y_0) + O(h\eta(\mathcal{S}_h^{[m]}, y_0) + h\varepsilon(\mathcal{S}_h^{[m]}, y_0)) \\ &= w^T D\varepsilon(\mathcal{S}_h^{[m]}, y_0) + O(h\eta(\mathcal{S}_h^{[m]}, y_0)) + O(h\varepsilon(\mathcal{S}_h^{[m]}, y_0)).\end{aligned}$$

Recall that  $D = (I - uw^T)(I - V + uu^T)^{-1}$ , then clearly  $w^T D = 0$  and we have

$$\eta(\mathcal{S}_h^{[m+1]}, y_0) = O(h\eta(\mathcal{S}_h^{[m]}, y_0)) + O(h\varepsilon(\mathcal{S}_h^{[m]}, y_0)).$$

Applying  $P(m)$ , we deduce that  $\eta(\mathcal{S}_h^{[m+1]}, y_0) = O(h^{m+p+2})$ .

For the  $\varepsilon$  map, we have that

$$\begin{aligned}\varepsilon(\mathcal{S}_h^{[m+1]}, y_0) &= \mathcal{M}_h \circ \mathcal{S}_h^{[m+1]}(y_0) - \mathcal{S}_h^{[m+1]} \circ \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[m+1]}(y_0) + u \circ \eta(\mathcal{S}_h^{[m+1]}, y_0), \\ &= \mathcal{M}_h \circ (\mathcal{S}_h^{[m]}(y_0) + D\varepsilon(\mathcal{S}_h^{[m]}, y_0) - u \circ \eta(\mathcal{S}_h^{[m]}, y_0)) - \\ &\quad \mathcal{S}_h^{[m]} \circ \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[m+1]}(y_0) - D\varepsilon(\mathcal{S}_h^{[m]}, \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[m+1]}(y_0)) + \\ &\quad u \circ \eta(\mathcal{S}_h^{[m]}, \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[m+1]}(y_0)) + O(h^{p+m+2}),\end{aligned}$$

using the result on the  $\eta$  map. Now, we approximate  $\mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[m+1]}(y_0) = y_0 + O(h)$  in the second argument of  $\eta$  and  $\varepsilon$ , and use the fact that Fréchet derivatives of  $\mathcal{M}_h$  and  $\mathcal{S}_h^{[m]}$  are given by  $V + O(h)$  and  $u + O(h)$  respectively to give

$$\begin{aligned}
\varepsilon(\mathcal{S}_h^{[m+1]}, y_0) &= \mathcal{M}_h \circ \mathcal{S}_h^{[m]}(y_0) + VD\varepsilon(\mathcal{S}_h^{[m]}, y_0) - Vu \circ \eta(\mathcal{S}_h^{[m]}, y_0) - \\
&\quad \mathcal{S}_h^{[m]} \circ \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[m]}(y_0) + D\varepsilon(\mathcal{S}_h^{[m]}, y_0) - u \circ \eta(\mathcal{S}_h^{[m]}, y_0) - \\
&\quad D\varepsilon(\mathcal{S}_h^{[m]}, y_0) + u \circ \eta(\mathcal{S}_h^{[m]}, y_0) + O(h^{p+m+2} + h\eta(\mathcal{S}_h^{[m]}, y_0) + h\varepsilon(\mathcal{S}_h^{[m]}, y_0)), \\
&= \mathcal{M}_h \circ \mathcal{S}_h^{[m]}(y_0) + VD\varepsilon(\mathcal{S}_h^{[m]}, y_0) - Vu \circ \eta(\mathcal{S}_h^{[m]}, y_0) - \\
&\quad \mathcal{S}_h^{[m]} \circ \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[m]}(y_0) - uw^T VD\varepsilon(\mathcal{S}_h^{[m]}, y_0) + uw^T Vu \circ \eta(\mathcal{S}_h^{[m]}, y_0) - \\
&\quad D\varepsilon(\mathcal{S}_h^{[m]}, y_0) + u \circ \eta(\mathcal{S}_h^{[m]}, y_0) + O(h^{p+m+2} + h\eta(\mathcal{S}_h^{[m]}, y_0) + h\varepsilon(\mathcal{S}_h^{[m]}, y_0)), \\
&= \varepsilon(\mathcal{S}_h^{[m]}, y_0) + VD\varepsilon(\mathcal{S}_h^{[m]}, y_0) - Vu \circ \eta(\mathcal{S}_h^{[m]}, y_0) - uw^T VD\varepsilon(\mathcal{S}_h^{[m]}, y_0) + \\
&\quad uw^T Vu \circ \eta(\mathcal{S}_h^{[m]}, y_0) - D\varepsilon(\mathcal{S}_h^{[m]}, y_0) + O(h^{p+m+2}),
\end{aligned}$$

where we have applied  $P(m)$ . Recalling pre-consistency condition  $Vu = u$ , this simplifies to

$$\varepsilon(\mathcal{S}_h^{[m+1]}, y_0) = (I - (I - V + uw^T V)D)\varepsilon(\mathcal{S}_h^{[m]}, y_0) + O(h^{p+m+2}).$$

We note that

$$\begin{aligned}
I - (I - V + uw^T V)D &= I - (I - V + uw^T V)(I - uw^T)(I - V + uu^T)^{-1}, \\
&= I - (I - V + uw^T V - uw^T)(I - V + uu^T)^{-1}, \\
&= I - (I - V + (uu^T - uu^T) + uw^T V - uw^T)(I - V + uu^T)^{-1}, \\
&= (u(w^T u)u^T - uw^T V + uw^T)(I - V + uu^T)^{-1}, \\
&= uw^T(uu^T - V + I)(I - V + uu^T)^{-1} = uw^T.
\end{aligned}$$

Thus,

$$\varepsilon(\mathcal{S}_h^{[m+1]}, y_0) = uw^T \varepsilon(\mathcal{S}_h^{[m]}, y_0) + O(h^{p+m+2}).$$

Finally, from the  $\varepsilon$  map definition:

$$\begin{aligned}
\mathcal{M}_h \circ \mathcal{S}_h^{[k]}(y_0) &= \mathcal{S}_h^{[k]} \circ \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[k]}(y_0) + \varepsilon(\mathcal{S}_h^{[k]}, y_0) - u \circ \eta(\mathcal{S}_h^{[k]}, y_0), \\
\Rightarrow \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[k]}(y_0) &= \mathcal{F}_h \circ \mathcal{S}_h^{[k]} \circ \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[k]}(y_0) + w^T \varepsilon(\mathcal{S}_h^{[k]}, y_0) - \\
&\quad w^T u \eta(\mathcal{S}_h^{[k]}, y_0) + O(h\eta(\mathcal{S}_h^{[k]}, y_0) + h\varepsilon(\mathcal{S}_h^{[k]}, y_0)), \\
&= \eta(\mathcal{S}_h^{[k]}, \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[k]}(y_0)) + \mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[k]}(y_0) + w^T \varepsilon(\mathcal{S}_h^{[k]}, y_0) + \\
&\quad \eta(\mathcal{S}_h^{[k]}, y_0) + O(h\eta(\mathcal{S}_h^{[k]}, y_0)) + O(h\varepsilon(\mathcal{S}_h^{[k]}, y_0)),
\end{aligned}$$

which, after using  $\mathcal{F}_h \circ \mathcal{M}_h \circ \mathcal{S}_h^{[k]}(y_0) = y_0 + O(h)$  in the second argument of  $\eta$ , we obtain

$$w^T \varepsilon(\mathcal{S}_h^{[k]}, y_0) = O(h\eta(\mathcal{S}_h^{[k]}, y_0) + h\varepsilon(\mathcal{S}_h^{[k]}, y_0)) = O(h^{p+m+2}),$$

after an application of  $P(m)$ . □

**Example 4.1.** Consider the pendulum problem given in Example 2.1. We test the iterative starting method with the Euler, modified Euler and symmetric starting methods. Note that each of these has a linear finishing method that satisfies  $\eta(\mathcal{S}_h^{[k]}, y_0) = 0, \forall k \geq 0$ . Thus, we only consider  $\varepsilon$ -convergence as given in Figure 2. The results indicate that the symmetric starting and finishing methods are the best choice for initialising the iterative starting method.

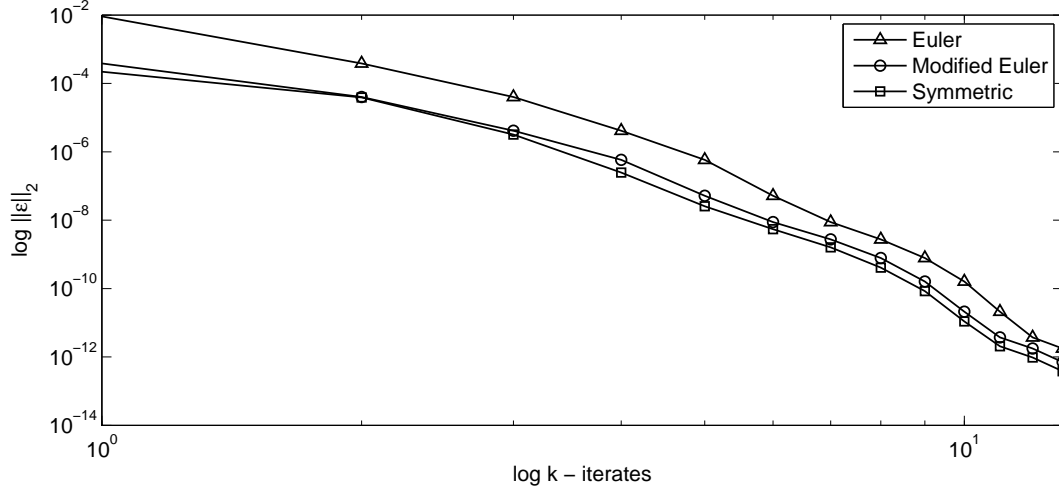


Figure 2:  $\varepsilon$ -convergence for the Leapfrog method on the simple pendulum. The Euler, modified Euler and symmetric starting and finishing methods are used to initialise the iterative starting method for  $0 \leq k \leq 13$ .

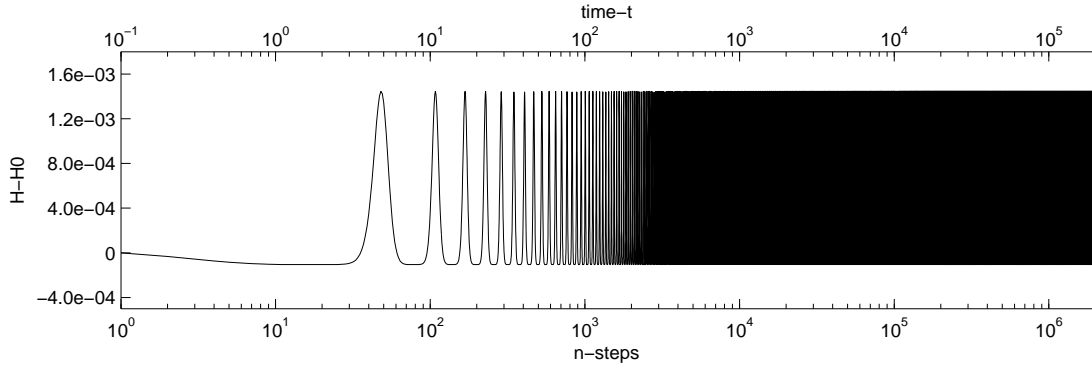


Figure 3: Error in the Hamiltonian for IVP (9). We fix  $h = 0.1$ ,  $t \in [0, 2 \times 10^5]$  and apply 13 iterations of the iterative starting method.

◇

## 5. Numerical Experiments

### 5.1. Simple Pendulum

Let us repeat the experiment in Example 2.1 with  $T = 10^5$ . The results are displayed in Figure 3 where, with 13 iterations of the iterative starting method, initialised using the symmetric starting and finishing methods, there is no observable parasitic growth.

### 5.2. Ablowitz-Ladik Discrete Nonlinear Schrödinger Equation

Consider the nonlinear cubic Schrödinger IVP,

$$iW_t = -W_{xx} - 2|W|^2W, \quad t \in \mathbb{R}, \quad x \in \left[-\frac{L}{2}, \frac{L}{2}\right], \quad (15)$$

$$W(x, 0) = W^0(x), \quad x \in \left[-\frac{L}{2}, \frac{L}{2}\right], \quad (16)$$

where  $L > 0$  is the domain length,  $W(x, t)$  is a complex scalar function and  $W^0(x)$  is given initial data. Taking periodic boundary conditions, we discretise equations (15)-(16) according to the Ablowitz-Ladik model: Given  $N \in \mathbb{N}$ , let  $\mathcal{I}_N := \{-(N-1), \dots, N\}$  and  $k := L/2N > 0$  denote the spatial step size. Then,

$$i \frac{dW_j}{dt} = -\frac{1}{k^2}(W_{j+1} - 2W_j + W_{j-1}) - |W_j|^2(W_{j+1} + W_{j-1}), \quad W_j(0) = W^0(jk), \quad j \in \mathcal{I}_N, \\ W_{-N}(t) = W_N(t), \quad W_{-(N-1)}(t) = W_{N+1}(t), \quad t \in \mathbb{R}.$$

This model is further simplified after applying the transformation  $V_j = W_j \exp(2ti/k^2)$ ,  $j \in \mathcal{I}_N$ :

$$i \frac{dV_j}{dt} = -\left(\frac{1}{k^2} + |V_j|^2\right)(V_{j+1} + V_{j-1}), \quad V_j(0) = W^0(jk), \quad j \in \mathcal{I}_N, \\ V_{-N}(t) = V_N(t), \quad V_{-(N-1)}(t) = V_{N+1}(t), \quad t \in \mathbb{R}. \quad (17)$$

System (17) is a completely integrable Poisson system. We introduce the vectors

$$V := \begin{bmatrix} V_{-(N-1)} \\ \vdots \\ V_N \end{bmatrix}, \quad p := \operatorname{Re}(V), \quad q := \operatorname{Im}(V), \quad z := \begin{bmatrix} p \\ q \end{bmatrix},$$

and the matrices

$$D(z) := I_{2N} + k^2 \cdot \operatorname{diag}\left(p_{-(N-1)}^2 + q_{-(N-1)}^2, \dots, p_N^2 + q_N^2\right), \quad B(z) := \begin{bmatrix} 0 & -D(z) \\ D(z) & 0 \end{bmatrix},$$

and re-write (17) as the Poisson system

$$\frac{dz}{dt} = B(z) \nabla_z G(z), \quad z(0) = z_0, \quad t \in \mathbb{R}, \quad (18)$$

where

$$G(z) = \frac{1}{k^2} \sum_{j \in \mathcal{I}_N} (p_j p_{j+1} + q_j q_{j+1}).$$

Techniques for integrating Poisson systems are discussed in [?, Chap. VII.4] and [?]. Here, we closely follow the standardisation approach of [?], where a Darboux transformation brings the system to Hamiltonian form (2), which we directly integrate with the Leapfrog method, as described below.

Consider the symmetric Darboux transformation suggested in [?, p. 274]:

$$\begin{cases} p_j = u_j \cdot \tau(k^2(u_j^2 + v_j^2)), \\ q_j = v_j \cdot \tau(k^2(u_j^2 + v_j^2)), \end{cases} \quad j \in \mathcal{I}_N, \quad \tau(x) = \sqrt{\frac{\exp(x) - 1}{x}}, \quad (19)$$

which has inverse

$$\begin{cases} u_j = p_j \cdot \sigma(k^2(p_j^2 + q_j^2)), \\ v_j = q_j \cdot \sigma(k^2(p_j^2 + q_j^2)), \end{cases} \quad j \in \mathcal{I}_N, \quad \sigma(x) = \sqrt{\frac{\ln(1+x)}{x}}.$$

Applying transformation (19) to (18) and setting

$$u := \begin{bmatrix} u_{-(N-1)} \\ \vdots \\ u_N \end{bmatrix}, \quad v := \begin{bmatrix} v_{-(N-1)} \\ \vdots \\ v_N \end{bmatrix}, \quad y := \begin{bmatrix} u \\ v \end{bmatrix},$$

we obtain the Hamiltonian system

$$\begin{aligned}\frac{dy}{dt} &= J^{-1} \nabla_y H(y), \quad y(0) = y_0, \quad t \in \mathbb{R}, \\ H(y) &= \frac{1}{k^2} \sum_{j \in \mathcal{I}_N} \tau(k^2(u_j^2 + v_j^2)) \tau(k^2(u_{j+1}^2 + v_{j+1}^2)) (v_j v_{j+1} + u_j u_{j+1}).\end{aligned}\tag{20}$$

For our experiment, we integrate (20) with the Leapfrog method initialised with 10 iterations of the iterative starting method, using the symmetric starting and finishing methods (7) and (8). Initial data is taken to be that of a single soliton,

$$W^0(x) = \exp(ix) \operatorname{sech}(x), \quad x \in \left[-\frac{L}{2}, \frac{L}{2}\right],\tag{21}$$

and the integration parameters are

$$N = 835, \quad L = 501, \quad k = 0.3, \quad h = 0.0145, \quad t \in [0, 10^5].$$

In Figure 4a we observe the propagation of the soliton over  $t \in [0, 100]$  and find that its shape remains approximately preserved. The Soliton is well-preserved over the longer interval, as verified in Figure 4b where  $t \in [99850, 99950]$ . The error in the Hamiltonian is given in Figure 4c, where good energy conservation is demonstrated for  $t \in [0, 10^5]$ .

## 6. Conclusion

Although parasitism afflicts time-symmetric and  $G$ -symplectic multivalued methods, the effects for many important problems can be relatively weak, and these effects may be attempted to be controlled. The iterative starting method described here has been shown to control the effects of parasitism, and to preserve geometrical features of the solution, for some non-trivial problems over very long time intervals. Our approach is low cost, compared say to taking intermittent implicit steps, since extra work is only required for the starting method. The fundamental geometric properties of the method appear unaffected in our numerical experiments, as they are by either restarts or the introduction of damping. Our approach also works for high order time-symmetric and  $G$ -symplectic multivalued methods. Another feature of the iterative starting method is that it may be used to automatically generate starting methods of maximal order for general linear methods, avoiding the necessity of explicitly constructing a suitable starting method. For conventional finite-time computations, only the preconsistency vectors  $u$  and  $w$  are needed to begin the iteration, and approximately  $p$  iterates are required to find a starting method of maximal order.

## Deleted Work

### Section 4.1

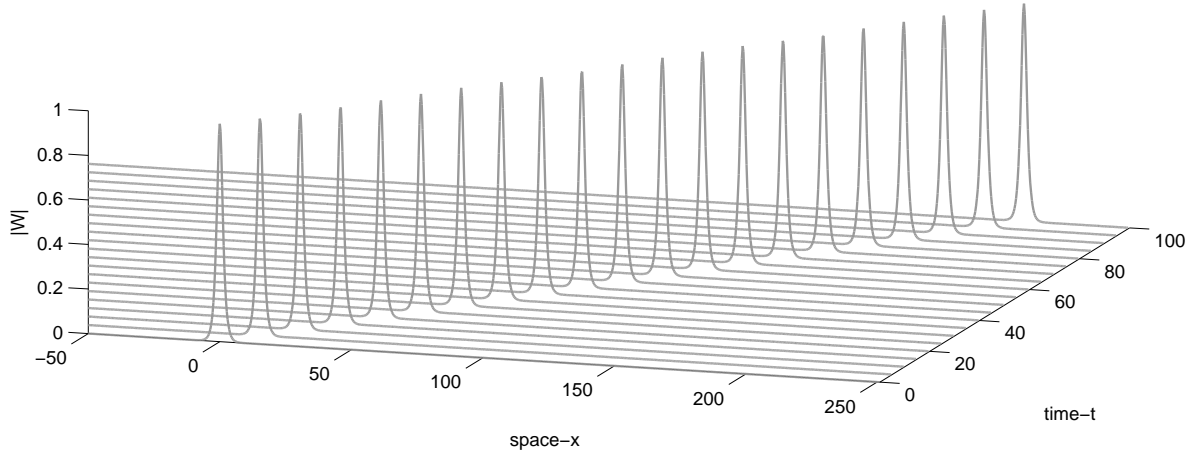
In what follows, we consider the case of a general linear method with  $r$  inputs. Furthermore, unless stated otherwise, we assume the corresponding finishing method is given by

$$\mathcal{F}_h := e_1^T = [1, 0, \dots, 0].$$

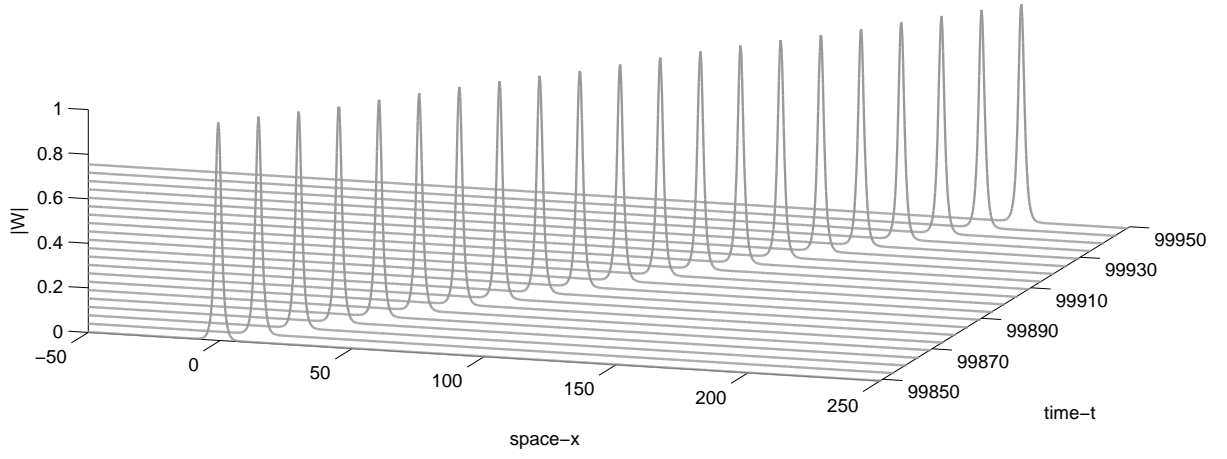
### 6.1. Diagonal Form

Further discussion requires that we consider GLMs that are in diagonal form, that is,  $V$  is diagonal. Suppose there is an invertible  $T \in \mathbb{R}^{r \times r}$  such that

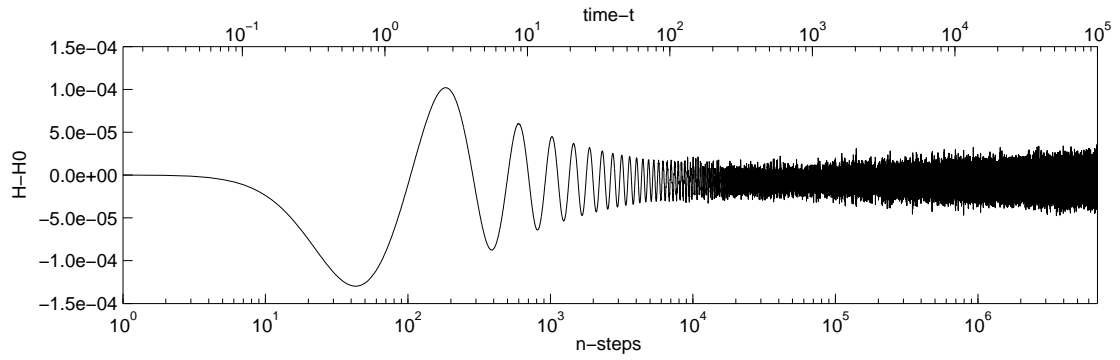
$$T^{-1}VT = \operatorname{diag}(1, \zeta_2, \dots, \zeta_r), \quad \zeta_2, \dots, \zeta_r \neq 1.$$



(a)



(b)



(c)

Figure 4: Results for the numerical integration of Hamiltonian IVP (20) and initial data (21). Leapfrog is initialised with 10 iterates of the iterative starting method using the symmetric starting and finishing methods. (a) Soliton evolution over interval  $t \in [0, 100]$ . (b) Soliton evolution over interval  $t \in [99850, 99950]$ . (c) Error in the Hamiltonian over interval  $t \in [0, 10^5]$ .

Then, we apply transformation  $T$  so that

$$\mathcal{F}_h \mathcal{M}_h^n \mathcal{S}_h(y_0) = (\mathcal{F}_h T)(T^{-1} \mathcal{M}_h T)^n (T^{-1} \mathcal{S}_h(y_0)) = \tilde{\mathcal{F}}_h \tilde{\mathcal{M}}_h^n \tilde{\mathcal{S}}_h(y_0),$$

where  $\tilde{\mathcal{M}}_h$  is an equivalent method in diagonal form and  $\tilde{\mathcal{S}}_h, \tilde{\mathcal{F}}_h$  are the corresponding transformed starting and finishing methods.

We note that the diagonalised form of the Leapfrog method is given by

$$\begin{bmatrix} A & UT \\ T^{-1}B & T^{-1}VT \end{bmatrix} = \left[ \begin{array}{c|cc} 0 & 1 & 1 \\ \hline 1 & 1 & 0 \\ 1 & 0 & -1 \end{array} \right],$$

where

$$T = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad T^{-1} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{bmatrix}.$$

Consequently, in the case of (7) and (8), the transformed symmetric starting and finishing methods are

$$\mathcal{S}_h(y_0) := \begin{bmatrix} y_0 \\ \frac{h}{2} f(y_0) \end{bmatrix}, \quad \mathcal{F}_h(y^{[n]}) := \begin{bmatrix} 1 & 0 \end{bmatrix} y^{[n]} = e_1^T y^{[n]},$$

where we have dropped the tildes.

#### Section 4.2

**Definition 6.1 (Starting Error Map).** The *starting error map*  $\varepsilon_h(\mathcal{S}_h) : X \rightarrow X^r$  is given as

$$\varepsilon_h(\mathcal{S}_h) := (I_X - \mathcal{S}_h \mathcal{F}_h) \mathcal{M}_h \mathcal{S}_h = (I - \mathcal{S}_h e_1^T) \mathcal{M}_h \mathcal{S}_h.$$

We see that this naturally defines an appropriate error map since should  $\mathcal{S}_h = \mathcal{S}_h^* + O(h^{N_0})$ , where  $N_0 \in \mathbb{N}$  is a sufficiently large truncation index, then

$$\varepsilon_h(\mathcal{S}_h) = \varepsilon_h(\mathcal{S}_h^* + O(h^{N_0})) = \varepsilon_h(\mathcal{S}_h^*) + O(h^{N_0} \varepsilon_h'(\mathcal{S}_h^*)),$$

where  $'$  denotes the Fréchet derivative. Since

$$\varepsilon_h(\mathcal{S}_h^*) = (I - \mathcal{S}_h^* e_1^T) \mathcal{M}_h \mathcal{S}_h^* = \mathcal{M}_h \mathcal{S}_h^* - \mathcal{S}_h^* e_1^T \mathcal{M}_h \mathcal{S}_h^* = \mathcal{M}_h \mathcal{S}_h^* - \mathcal{S}_h^* \Phi_h = 0,$$

it follows that  $\varepsilon_h(\mathcal{S}_h) = O(h^{N_0})$ .

**Definition 6.2 (Iterative starting method).** We define the *iterative starting method* as follows:

$$\begin{aligned} \mathcal{S}_h^{[k+1]} &= \mathcal{S}_h^{[k]} + D \varepsilon_h(\mathcal{S}_h^{[k]}), \quad \forall k \geq 0, \\ \mathcal{S}_h^{[0]} &= \mathcal{S}_h, \end{aligned}$$

where  $D = \text{diag}\left(0, \frac{1}{1-\zeta_2}, \dots, \frac{1}{1-\zeta_r}\right)$ .

**Lemma 6.1.** The map  $\varepsilon_h$  satisfies  $e_1^T \varepsilon_h(\mathcal{S}_h^{[k]}) = 0, \forall k \geq 0$ .

*Proof.* Noting that  $e_1^T D = 0$ , we find

$$\begin{aligned} e_1^T \mathcal{S}_h^{[k]} &= e_1^T \mathcal{S}_h^{[k-1]} + e_1^T D \varepsilon_h(\mathcal{S}_h^{[k-1]}) = e_1^T \mathcal{S}_h^{[k-1]}, \\ \Rightarrow e_1^T \mathcal{S}_h^{[k]} &= e_1^T \mathcal{S}_h^{[k-1]} = \dots = e_1^T \mathcal{S}_h^{[0]} = I, \end{aligned}$$

since  $\mathcal{F}_h \mathcal{S}_h = e_1^T \mathcal{S}_h = I$ . It now follows that

$$e_1^T \varepsilon_h(\mathcal{S}_h^{[k]}) = e_1^T (I - \mathcal{S}_h^{[k]} e_1^T) \mathcal{M}_h \mathcal{S}_h^{[k]} = (e_1^T - e_1^T) \mathcal{M}_h \mathcal{S}_h^{[k]} = 0.$$

□



## Section 5

In the following experiments, we use the symmetric starting and finishing methods (7) and (8) as the basis of the iterative starting method of Definition ??, where

$$D = \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{2} \end{bmatrix}, \quad \text{or in original coordinates,} \quad TDT^{-1} = \begin{bmatrix} \frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{1}{4} \end{bmatrix}.$$

### *Euler and modified Euler starting methods*

A sufficiently accurate starting approximation is given by the classical **Euler starting method**:

$$\begin{aligned} U_1 &= y_0 + hf(y_0), \\ U_0 &= y_0. \end{aligned} \tag{22}$$

Gragg [?] proved that, with the Euler starting method, the global error expansion for the Leapfrog method contains only even powers of  $h$ ; such expansions are characteristic of time-symmetric multistep methods [?, pp. 415-416].

**Example 6.1.** Consider the simple pendulum problem:

$$\frac{d}{dt} \begin{bmatrix} p(t) \\ q(t) \end{bmatrix} = \begin{bmatrix} -\sin(q(t)) \\ p(t) \end{bmatrix}, \quad \begin{bmatrix} p(0) \\ q(0) \end{bmatrix} = \begin{bmatrix} 1.0 \\ 2.0 \end{bmatrix}, \quad t \in [0, 4]. \tag{23}$$

We note that this is a Hamiltonian IVP, with a separable Hamiltonian of the form

$$H(q, p) = \frac{1}{2}p^2 - \cos(q).$$

We solve IVP (9) with a fixed time-step of  $h = 0.1$ . The Hamiltonian error,  $H(q_n, p_n) - H(q_0, p_0)$ , is plotted in Figure 1a. This experiment shows that the Hamiltonian is almost constant for about 10 time-steps. However, subsequently, the growth of a parasitic mode of the Leapfrog method overwhelms the principal component of the numerical solution. A similar experiment is performed in [?] where parasitism is also observed.

◇

The second starting method we consider is the **modified Euler starting method**. Here,  $U_1 = \varphi_h(y_0) + O(h^3)$ :

$$\begin{aligned} U_1 &= y_0 + \frac{h}{2}f(y_0) + \frac{h}{2}f(y_0 + hf(y_0)), \\ U_0 &= y_0. \end{aligned} \tag{24}$$

**Example 6.2.** We repeat Example ?? over the extended interval of  $t \in [0, 2000]$ , initialising Leapfrog with the modified Euler starting method (6). The numerical results are displayed in Figure 1b. We find that the Hamiltonian is quite well-preserved for  $t \in [0, 50]$ . However, subsequently, parasitic instability begins to dominate the Hamiltonian error.

◇

The previous example suggests that a sufficiently high order approximation,  $U_1$ , to  $\varphi_h(y_0)$  may extend the interval of good Hamiltonian preservation. However, experiments using RK4, in which  $U_1$  is computed to an accuracy of  $O(h^5)$  reveal no substantial improvement on the results in Example ??.

### A simple symmetric starting method

Here, we consider a more general starting method in which  $U_n$  does not necessarily approximate  $y(nh)$ . In such a framework, we need a finishing method that maps the numerical solution to an approximation of  $y(nh)$ . In particular, we construct a starting method that explicitly respects the time-symmetry of the Leapfrog method. Below, we consider the reversibility of the numerical method as a whole: starting method, main method and finishing method.

Let  $y^{[n]} := [U_{n+1}^T, U_n^T]^T$ . The map associated with the Leapfrog method is  $\mathcal{M}_h : X^2 \rightarrow X^2$  such that  $y^{[n+1]} = \mathcal{M}_h y^{[n]}$ . In detail,

$$\begin{aligned} y^{[n+1]} &= 2hf(Y)e_1 + Vy^{[n]}, \\ Y &= e_1^T y^{[n]}, \end{aligned} \quad e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad V = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

where the Kronecker product is implied.

**Lemma 6.2.**

$$\mathcal{M}_h = L\mathcal{M}_{-h}^{-1}L, \quad \text{for} \quad L = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

*Proof.*  $\mathcal{M}_h^{-1}$  is the map  $y^{[n+1]} \mapsto y^{[n]}$ . Now, using  $V^{-1} = V$ ,

$$\begin{aligned} y^{[n]} &= -2hf(Y)V^{-1}e_1 + V^{-1}y^{[n+1]}, \\ &= 2(-h)f(Y)e_2 + Vy^{[n+1]}. \\ Y &= e_1^T(2(-h)f(Y)e_2 + Vy^{[n+1]}), \\ &= e_2^T y^{[n+1]}. \end{aligned}$$

Note that,  $L\mathcal{M}_{-h}^{-1}L$  is the map  $Ly^{[n+1]} \mapsto Ly^{[n]}$  for  $h \longleftrightarrow -h$ . Using  $Le_2 = e_1, LV^{-1}L = V$ , we conclude that

$$\begin{aligned} Ly^{[n]} &= 2hf(Y)e_1 + V(Ly^{[n+1]}), \\ Y &= e_1^T(Ly^{[n+1]}). \end{aligned}$$

But this describes the same map as  $\mathcal{M}_h$ . □

As Leapfrog is a two-step method, any starting method  $\mathcal{S}_h$  is a map of the form  $\mathcal{S}_h : X \rightarrow X^2$ . In [?], a starting method is said to be *symmetric* if

$$L\mathcal{S}_{-h} = \mathcal{S}_h. \tag{25}$$

This definition is partially justified by identity (??) below. Here, we consider

$$\mathcal{S}_h(y_0) := \begin{bmatrix} y_0 + \frac{h}{2}f(y_0) \\ y_0 - \frac{h}{2}f(y_0) \end{bmatrix}, \tag{26}$$

which satisfies (??).

Similarly, the map associated with a Leapfrog finishing method is of the form  $\mathcal{F}_h : X^2 \rightarrow X$ , such that  $\mathcal{F}_h(y^{[n]}) \approx y(nh)$  and  $\mathcal{F}_h\mathcal{S}_h = I_X$ , where  $\mathcal{S}_h$  is the corresponding starting method. A finishing method is said to be *symmetric* if  $\mathcal{F}_{-h}L = \mathcal{F}_h$ . Here, a suitable, symmetric finishing method corresponding to  $\mathcal{S}_h$  in (7) is

$$\mathcal{F}_h(y^{[n]}) = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix} y^{[n]}. \tag{27}$$

Note now that the numerical method as a whole is described by the map  $\mathcal{F}_h \mathcal{M}_h^n \mathcal{S}_h(y_0)$ . By Lemma ?? and the symmetry conditions for  $\mathcal{S}_h$  and  $\mathcal{F}_h$ , we confirm that this map is reversible, i.e.

$$\mathcal{F}_h \mathcal{M}_h^n \mathcal{S}_h(y_0) = \mathcal{F}_{-h} \mathcal{M}_{-h}^{-n} \mathcal{S}_{-h}(y_0). \quad (28)$$

This follows since

$$\mathcal{F}_{-h} \mathcal{M}_{-h}^{-n} \mathcal{S}_{-h}(y_0) = (\mathcal{F}_{-h} L)(L \mathcal{M}_{-h}^{-n} L)(L \mathcal{S}_{-h})(y_0) = \mathcal{F}_h (L \mathcal{M}_{-h}^{-1} L)^n \mathcal{S}_h(y_0) = \mathcal{F}_h \mathcal{M}_h^n \mathcal{S}_h(y_0).$$

It can be verified that this combination of starting and finishing methods maintains second-order accuracy and implies a global error expansion in even powers of  $h$ . A treatment of time-symmetric general linear methods can found in [?] and [?, Chap. XV.8.2]; the time-symmetry of starting and finishing methods is explored in the former. We note that, as shown in [? ?], the Leapfrog method with Euler starting method and conventional finishing method is symmetric as a whole, even though  $\mathcal{S}_h$  and  $\mathcal{F}_h$  are not symmetric in the sense defined above.

**Example 6.3.** We repeat Example ??, initialising with (7) and finishing with (8). The results are given in Figure 1c. In comparison to the previous example, an extended interval of good preservation is observed. However, parasitism ultimately dominates.

◇